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Triaquatris(nitrato-κ^2O,O')lanthanum(III) 4,4′-bipyridine disolvate

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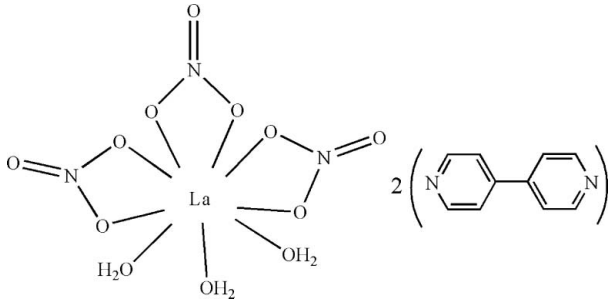
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.028; wR factor = 0.082; data-to-parameter ratio = 16.1.

The La^{III} atom in the title complex, $[La(NO_3)_3(H_2O)_3]\cdot 2C_{10}H_8N_2$, is irregularly coordinated by three O atoms of three water molecules and six O atoms of three NO_3^- ligands. This mononuclear complex is further extended into a supramolecular network structure *via* O—H···O and O—H···N hydrogen bonds.

Related literature

For related structures, see: Benelli *et al.* (1992); Daiguebonne *et al.* (2000); Farrugia *et al.* (2000); Miller & Drillon (2001*a*,*b*, 2002); Modolo & Odoj (1998). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[La(NO_3)_3(H_2O)_3]\cdot 2C_{10}H_8N_2$
M_r = 691.36
Monoclinic, $P2_1/n$
a = 7.970 (2) Å
b = 20.781 (2) Å
c = 16.401 (3) Å
β = 102.298 (7)°
V = 2654.1 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.68 mm^{-1}
T = 273 (2) K
0.49 × 0.38 × 0.30 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.493, T_{max} = 0.632
17534 measured reflections
6212 independent reflections
5157 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.082
S = 0.99
6212 reflections
386 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

La1—O1	2.357 (2)	La1—O7	2.520 (2)
La1—O2	2.389 (2)	La1—O9	2.496 (3)
La1—O3	2.380 (2)	La1—O10	2.495 (2)
La1—O4	2.519 (2)	La1—O12	2.521 (3)
La1—O6	2.446 (2)		
O1—La1—O2	85.67 (8)	O3—La1—O9	125.16 (8)
O1—La1—O3	82.86 (9)	O3—La1—O10	145.23 (8)
O1—La1—O4	150.97 (9)	O3—La1—O12	151.29 (9)
O1—La1—O6	145.57 (7)	O4—La1—O6	51.31 (7)
O1—La1—O7	72.18 (8)	O4—La1—O7	118.73 (7)
O1—La1—O9	84.03 (8)	O4—La1—O9	124.26 (7)
O1—La1—O10	128.55 (9)	O4—La1—O10	69.93 (8)
O1—La1—O12	78.13 (8)	O4—La1—O12	113.28 (7)
O2—La1—O3	83.34 (9)	O6—La1—O7	73.63 (7)
O2—La1—O4	73.08 (8)	O6—La1—O9	77.50 (8)
O2—La1—O6	124.35 (8)	O6—La1—O10	75.77 (8)
O2—La1—O7	150.27 (8)	O6—La1—O12	122.93 (8)
O2—La1—O9	147.91 (9)	O7—La1—O9	50.69 (8)
O2—La1—O10	84.70 (10)	O7—La1—O10	124.58 (9)
O2—La1—O12	74.00 (9)	O7—La1—O12	118.61 (8)
O3—La1—O4	75.36 (8)	O9—La1—O10	78.28 (9)
O3—La1—O6	84.41 (9)	O9—La1—O12	74.15 (9)
O3—La1—O7	74.62 (8)	O10—La1—O12	50.65 (8)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2B···N6	0.86 (4)	1.84 (4)	2.668 (4)	161 (5)
O1—H1A···N7	0.87 (3)	1.87 (3)	2.736 (4)	173 (5)
O1—H1B···N5^{i}	0.88 (3)	1.87 (3)	2.747 (3)	172 (4)
O3—H3A···N4^{ii}	0.86 (5)	2.08 (6)	2.684 (3)	128 (6)
O2—H2A···O8^{iii}	0.86 (3)	2.21 (2)	3.002 (4)	154 (5)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+2, -y+1, -z+1$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2414).

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supplementary materials

Acta Cryst. (2007). E**63**, m2715-m2716 [**doi:10.1107/S1600536807049227**]

Triaquatris(nitrato-κ^2O,O')lanthanum(III) 4,4'-bipyridine disolvate

N.-G. Li, R.-M. Tao and B.-F. Fu

Comment

Molecular magnetic compounds, such as molecular ferro- and ferrimagnets, organic magnets, single-molecule magnets and high-spin molecules, have recently attracted attention (Miller & Drillon, 2001*a*,b, 2002). Owing to Lanthanide metals unique physical and chemical properties, Lanthanide complexes play an important role in special materials having optical, electronic, magnetic and biological importance (Benelli *et al.*, 1992; Daiguebonne *et al.*, 2000; Farrugia *et al.*, 2000). More importantly, since the removal of lanthanides from radioactive highlevel liquid waste (HLLW) has been shown to improve the transmutation of long-lived transuranic elements to shortlived or even stable nuclides (Modolo & Odoj, 1998), the coordination chemistry of the 4f metals continues to attract interest. We report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The irregular nine-coordinate environment of the La atom is completed by the three O atoms of three water molecules and six O atoms of three NO_3^- (Table 1). The La—O bond lengths are in the range 2.357 (2) to 2.389 (2) Å for the O atoms in water molecules. The La—O bond length are in the range 2.446 (2) to 2.521 (3) Å for NO_3^-. The O—H···O and O—H···N hydrogen bonds link the mononuclear complex into a supramolecular network structure (Fig. 2).

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Lanthanum trinitrate hexahydrate (324.9 mg, 1 mmol), 4,4'-bipyridyl (312 mg, 2 mmol), and distilled water (10 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure for 7 d at 453 K and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colourless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H atoms of water were located from difference Fourier syntheses and refined with restraints to the O—H distances and the H—O—H angles. The remaining H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

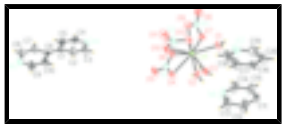


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

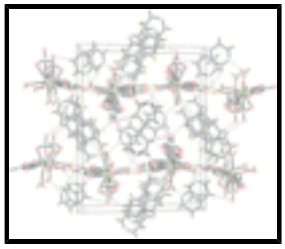


Fig. 2. Packing diagram for (I) showing hydrogen bonds as dashed lines.

Triaquatris(nitrato-κ^2*O*,*O*')lanthanum(III) 4,4'-bipyridine disolvate

Crystal data

$[La(NO_3)_3(H_2O)_3]\cdot 2C_{10}H_8N_2$	F_{000} = 1376
M_r = 691.36	D_x = 1.730 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 12612 reflections
a = 7.970 (2) Å	θ = 2.7–28.2º
b = 20.781 (2) Å	μ = 1.68 mm^{-1}
c = 16.401 (3) Å	T = 273 (2) K
β = 102.298 (7)º	Plane, colourless
V = 2654.1 (9) Å^3	0.49 × 0.38 × 0.30 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	6212 independent reflections
Radiation source: fine-focus sealed tube	5157 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.049
T = 273(2) K	θ_{max} = 27.9º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→9
T_{min} = 0.493, T_{max} = 0.632	k = −27→27
17534 measured reflections	l = −21→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.028	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.082	$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.02P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max}$ = 0.001

6212 reflections	$\Delta\rho_{max}$ = 0.93 e Å^{-3}
386 parameters	$\Delta\rho_{min}$ = −0.44 e Å^{-3}
9 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0078 (4)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
La1	0.438501 (17)	0.278104 (6)	0.274724 (8)	0.03525 (7)
O1	0.4038 (3)	0.16647 (11)	0.29063 (15)	0.0682 (6)
O2	0.3592 (3)	0.25771 (12)	0.12823 (14)	0.0633 (6)
O3	0.7158 (3)	0.24651 (12)	0.25735 (16)	0.0638 (5)
O4	0.5438 (3)	0.37217 (10)	0.20267 (13)	0.0609 (5)
O5	0.6599 (4)	0.45664 (11)	0.26918 (16)	0.0908 (8)
O6	0.5855 (3)	0.37538 (10)	0.33652 (13)	0.0661 (6)
O7	0.6014 (3)	0.24707 (11)	0.41840 (13)	0.0609 (5)
O8	0.4964 (4)	0.24869 (15)	0.52941 (14)	0.0876 (7)
O9	0.3482 (3)	0.28523 (11)	0.41114 (15)	0.0714 (7)
O10	0.2132 (3)	0.36337 (11)	0.24552 (19)	0.0880 (9)
O11	−0.0605 (3)	0.34686 (15)	0.2212 (3)	0.1190 (12)
O12	0.1162 (3)	0.26681 (11)	0.24108 (17)	0.0656 (6)
N1	0.5981 (3)	0.40299 (11)	0.26873 (16)	0.0597 (6)
N2	0.4822 (4)	0.26057 (14)	0.45497 (16)	0.0598 (6)
N3	0.0856 (3)	0.32594 (16)	0.23588 (19)	0.0714 (8)
N4	1.0674 (4)	0.83522 (15)	0.6463 (2)	0.0777 (8)
N5	0.5812 (4)	1.08020 (14)	0.4039 (2)	0.0745 (8)
N6	0.5071 (4)	0.16530 (13)	0.0550 (2)	0.0805 (9)
N7	0.1989 (5)	0.08374 (17)	0.1836 (2)	0.0953 (11)
C1	0.8645 (4)	0.92986 (13)	0.55189 (18)	0.0512 (6)
C2	0.8741 (7)	0.86922 (18)	0.5232 (3)	0.1192 (19)
H2	0.8094	0.8577	0.4711	0.143*
C3	0.9790 (8)	0.8245 (2)	0.5706 (4)	0.140 (2)
H3	0.9877	0.7841	0.5474	0.168*
C4	1.0546 (6)	0.8937 (2)	0.6742 (2)	0.1056 (16)

H4	1.1165	0.9035	0.7275	0.127*
C5	0.9553 (6)	0.9420 (2)	0.6299 (2)	0.0953 (14)
H5	0.9511	0.9825	0.6535	0.114*
C6	0.7631 (4)	0.98137 (13)	0.50085 (17)	0.0508 (6)
C7	0.7416 (6)	1.04134 (17)	0.5322 (2)	0.0892 (13)
H7	0.7861	1.0501	0.5882	0.107*
C8	0.6555 (6)	1.08824 (18)	0.4818 (3)	0.0969 (14)
H8	0.6496	1.1289	0.5048	0.116*
C9	0.5993 (6)	1.0231 (2)	0.3740 (3)	0.1067 (16)
H9	0.5495	1.0159	0.3182	0.128*
C10	0.6870 (6)	0.97233 (19)	0.4189 (2)	0.0951 (14)
H10	0.6939	0.9327	0.3935	0.114*
C11	0.5049 (4)	0.03433 (14)	0.0113 (2)	0.0618 (8)
C12	0.4307 (6)	0.08096 (19)	−0.0440 (3)	0.1083 (18)
H12	0.3770	0.0696	−0.0981	0.130*
C13	0.4354 (6)	0.14446 (19)	−0.0197 (3)	0.1069 (16)
H13	0.3841	0.1747	−0.0591	0.128*
C14	0.5861 (6)	0.12116 (19)	0.1079 (3)	0.1000 (14)
H14	0.6447	0.1345	0.1604	0.120*
C15	0.5858 (6)	0.05579 (18)	0.0888 (2)	0.0942 (13)
H15	0.6407	0.0266	0.1287	0.113*
C16	0.0409 (5)	0.01783 (16)	0.0385 (2)	0.0707 (9)
C17	0.0126 (6)	0.08216 (18)	0.0486 (3)	0.1009 (15)
H17	−0.0606	0.1051	0.0069	0.121*
C18	0.0926 (7)	0.1122 (2)	0.1202 (3)	0.1071 (16)
H18	0.0714	0.1558	0.1252	0.129*
C19	0.2228 (6)	0.0216 (2)	0.1734 (3)	0.0981 (14)
H19	0.2957	−0.0003	0.2163	0.118*
C20	0.1478 (5)	−0.01283 (19)	0.1041 (2)	0.0838 (11)
H20	0.1689	−0.0567	0.1012	0.101*
H1A	0.332 (5)	0.1409 (16)	0.259 (2)	0.15 (2)*
H2A	0.265 (4)	0.268 (2)	0.095 (2)	0.13 (2)*
H3A	0.798 (6)	0.220 (3)	0.256 (4)	0.22 (4)*
H1B	0.457 (4)	0.1409 (14)	0.3308 (17)	0.096 (13)*
H2B	0.420 (5)	0.235 (2)	0.102 (2)	0.12 (2)*
H3B	0.752 (9)	0.272 (2)	0.298 (3)	0.17 (3)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.03376 (10)	0.02805 (9)	0.03997 (10)	0.00117 (5)	−0.00108 (6)	0.00237 (5)
O1	0.0846 (16)	0.0435 (11)	0.0659 (13)	−0.0056 (11)	−0.0074 (12)	0.0100 (10)
O2	0.0707 (16)	0.0557 (12)	0.0572 (13)	0.0119 (12)	−0.0006 (12)	−0.0075 (10)
O3	0.0490 (13)	0.0588 (13)	0.0806 (16)	0.0109 (11)	0.0071 (11)	0.0137 (12)
O4	0.0658 (13)	0.0535 (12)	0.0579 (11)	−0.0069 (10)	0.0008 (9)	0.0015 (9)
O5	0.119 (2)	0.0491 (13)	0.0964 (18)	−0.0300 (14)	0.0049 (16)	0.0110 (12)
O6	0.0860 (16)	0.0499 (11)	0.0570 (12)	−0.0137 (11)	0.0030 (11)	0.0040 (9)
O7	0.0606 (13)	0.0597 (12)	0.0582 (12)	0.0041 (11)	0.0026 (10)	0.0033 (10)

O8	0.103 (2)	0.1063 (19)	0.0494 (13)	−0.0033 (19)	0.0070 (13)	0.0055 (13)
O9	0.0649 (16)	0.0839 (17)	0.0631 (14)	0.0097 (11)	0.0085 (12)	0.0015 (11)
O10	0.0500 (14)	0.0512 (13)	0.159 (3)	0.0043 (11)	0.0142 (15)	0.0212 (15)
O11	0.0488 (15)	0.105 (2)	0.201 (4)	0.0224 (15)	0.0232 (18)	0.063 (2)
O12	0.0519 (12)	0.0577 (13)	0.0834 (15)	−0.0018 (11)	0.0057 (11)	0.0117 (11)
N1	0.0667 (16)	0.0434 (12)	0.0624 (15)	−0.0051 (12)	−0.0007 (12)	0.0084 (11)
N2	0.0672 (18)	0.0585 (14)	0.0497 (14)	−0.0027 (13)	0.0036 (13)	−0.0018 (11)
N3	0.0442 (15)	0.0682 (19)	0.101 (2)	0.0091 (13)	0.0128 (14)	0.0302 (15)
N4	0.0612 (17)	0.079 (2)	0.094 (2)	0.0176 (15)	0.0190 (15)	0.0369 (17)
N5	0.0684 (19)	0.0596 (17)	0.091 (2)	0.0056 (14)	0.0072 (16)	0.0223 (15)
N6	0.081 (2)	0.0556 (16)	0.094 (2)	0.0138 (15)	−0.0054 (17)	−0.0187 (15)
N7	0.121 (3)	0.079 (2)	0.078 (2)	−0.040 (2)	0.003 (2)	−0.0023 (17)
C1	0.0459 (15)	0.0493 (15)	0.0585 (16)	0.0016 (12)	0.0116 (12)	0.0107 (12)
C2	0.155 (4)	0.057 (2)	0.113 (3)	0.034 (3)	−0.046 (3)	−0.013 (2)
C3	0.176 (6)	0.062 (3)	0.146 (4)	0.044 (3)	−0.046 (4)	−0.007 (3)
C4	0.128 (4)	0.115 (3)	0.064 (2)	0.066 (3)	−0.002 (2)	0.008 (2)
C5	0.120 (3)	0.089 (3)	0.066 (2)	0.046 (3)	−0.007 (2)	−0.0045 (19)
C6	0.0483 (15)	0.0460 (14)	0.0572 (15)	−0.0010 (12)	0.0093 (12)	0.0085 (11)
C7	0.131 (4)	0.0546 (19)	0.068 (2)	0.023 (2)	−0.011 (2)	−0.0029 (16)
C8	0.136 (4)	0.055 (2)	0.086 (3)	0.029 (2)	−0.007 (3)	0.0037 (18)
C9	0.133 (4)	0.093 (3)	0.074 (2)	0.026 (3)	−0.023 (2)	0.009 (2)
C10	0.130 (4)	0.066 (2)	0.070 (2)	0.022 (2)	−0.021 (2)	−0.0011 (18)
C11	0.0572 (18)	0.0529 (17)	0.0697 (19)	0.0152 (15)	0.0012 (14)	−0.0123 (14)
C12	0.132 (4)	0.066 (2)	0.097 (3)	0.028 (2)	−0.044 (3)	−0.022 (2)
C13	0.128 (4)	0.056 (2)	0.108 (3)	0.024 (2)	−0.040 (3)	−0.011 (2)
C14	0.133 (4)	0.069 (2)	0.081 (2)	0.028 (2)	−0.016 (2)	−0.0215 (19)
C15	0.128 (4)	0.064 (2)	0.076 (2)	0.026 (2)	−0.012 (2)	−0.0105 (18)
C16	0.081 (2)	0.0626 (19)	0.0657 (19)	−0.0302 (17)	0.0092 (17)	0.0075 (15)
C17	0.145 (4)	0.058 (2)	0.082 (3)	−0.026 (2)	−0.014 (3)	0.0054 (18)
C18	0.158 (4)	0.064 (2)	0.087 (3)	−0.032 (3)	−0.003 (3)	0.005 (2)
C19	0.109 (3)	0.088 (3)	0.083 (3)	−0.018 (3)	−0.012 (2)	0.007 (2)
C20	0.089 (3)	0.072 (2)	0.080 (2)	−0.020 (2)	−0.005 (2)	0.0048 (19)

Geometric parameters (Å, °)

La1—O1	2.357 (2)	C1—C6	1.487 (4)
La1—O2	2.389 (2)	C2—C3	1.375 (5)
La1—O3	2.380 (2)	C2—H2	0.9300
La1—O4	2.519 (2)	C3—H3	0.9300
La1—O6	2.446 (2)	C4—C5	1.384 (5)
La1—O7	2.520 (2)	C4—H4	0.9300
La1—O9	2.496 (3)	C5—H5	0.9300
La1—O10	2.495 (2)	C6—C10	1.364 (4)
La1—O12	2.521 (3)	C6—C7	1.373 (4)
O1—H1A	0.87 (3)	C7—C8	1.365 (5)
O1—H1B	0.88 (3)	C7—H7	0.9300
O2—H2A	0.86 (3)	C8—H8	0.9300
O2—H2B	0.86 (4)	C9—C10	1.388 (5)
O3—H3A	0.86 (5)	C9—H9	0.9300

O3—H3B	0.85 (5)	C10—H10	0.9300
O4—N1	1.254 (3)	C11—C15	1.371 (5)
O5—N1	1.219 (3)	C11—C12	1.372 (5)
O6—N1	1.274 (3)	C11—C11^{i}	1.472 (6)
O7—N2	1.259 (3)	C12—C13	1.377 (5)
O8—N2	1.227 (3)	C12—H12	0.9300
O9—N2	1.262 (4)	C13—H13	0.9300
O10—N3	1.263 (4)	C14—C15	1.394 (5)
O11—N3	1.218 (3)	C14—H14	0.9300
O12—N3	1.252 (3)	C15—H15	0.9300
N4—C3	1.310 (6)	C16—C17	1.372 (5)
N4—C4	1.311 (5)	C16—C20	1.377 (5)
N5—C8	1.299 (5)	C16—C16^{ii}	1.490 (6)
N5—C9	1.302 (5)	C17—C18	1.363 (5)
N6—C13	1.312 (5)	C17—H17	0.9300
N6—C14	1.325 (5)	C18—H18	0.9300
N7—C19	1.322 (5)	C19—C20	1.368 (5)
N7—C18	1.331 (5)	C19—H19	0.9300
C1—C5	1.353 (4)	C20—H20	0.9300
C1—C2	1.353 (4)		
O1—La1—O2	85.67 (8)	O7—N2—O9	116.9 (3)
O1—La1—O3	82.86 (9)	O11—N3—O12	121.9 (3)
O1—La1—O4	150.97 (9)	O11—N3—O10	121.0 (3)
O1—La1—O6	145.57 (7)	O12—N3—O10	117.1 (3)
O1—La1—O7	72.18 (8)	C3—N4—C4	115.0 (3)
O1—La1—O9	84.03 (8)	C8—N5—C9	115.0 (3)
O1—La1—O10	128.55 (9)	C13—N6—C14	115.8 (3)
O1—La1—O12	78.13 (8)	C19—N7—C18	114.8 (3)
O2—La1—O3	83.34 (9)	C5—C1—C2	116.4 (3)
O2—La1—O4	73.08 (8)	C5—C1—C6	121.0 (3)
O2—La1—O6	124.35 (8)	C2—C1—C6	122.6 (3)
O2—La1—O7	150.27 (8)	C1—C2—C3	120.4 (4)
O2—La1—O9	147.91 (9)	C1—C2—H2	119.8
O2—La1—O10	84.70 (10)	C3—C2—H2	119.8
O2—La1—O12	74.00 (9)	N4—C3—C2	124.1 (4)
O3—La1—O4	75.36 (8)	N4—C3—H3	118.0
O3—La1—O6	84.41 (9)	C2—C3—H3	118.0
O3—La1—O7	74.62 (8)	N4—C4—C5	124.5 (4)
O3—La1—O9	125.16 (8)	N4—C4—H4	117.7
O3—La1—O10	145.23 (8)	C5—C4—H4	117.7
O3—La1—O12	151.29 (9)	C1—C5—C4	119.5 (4)
O4—La1—O6	51.31 (7)	C1—C5—H5	120.2
O4—La1—O7	118.73 (7)	C4—C5—H5	120.2
O4—La1—O9	124.26 (7)	C10—C6—C7	115.4 (3)
O4—La1—O10	69.93 (8)	C10—C6—C1	122.0 (3)
O4—La1—O12	113.28 (7)	C7—C6—C1	122.6 (3)
O6—La1—O7	73.63 (7)	C8—C7—C6	120.5 (3)
O6—La1—O9	77.50 (8)	C8—C7—H7	119.7

O6—La1—O10	75.77 (8)	C6—C7—H7	119.7
O6—La1—O12	122.93 (8)	N5—C8—C7	124.7 (4)
O7—La1—O9	50.69 (8)	N5—C8—H8	117.7
O7—La1—O10	124.58 (9)	C7—C8—H8	117.7
O7—La1—O12	118.61 (8)	N5—C9—C10	125.2 (4)
O9—La1—O10	78.28 (9)	N5—C9—H9	117.4
O9—La1—O12	74.15 (9)	C10—C9—H9	117.4
O10—La1—O12	50.65 (8)	C6—C10—C9	119.0 (4)
O1—La1—H3B	94.2 (13)	C6—C10—H10	120.5
O2—La1—H3B	101.0 (9)	C9—C10—H10	120.5
O6—La1—H3B	66.1 (8)	C15—C11—C12	115.8 (3)
O10—La1—H3B	137.3 (13)	C15—C11—C11^{i}	122.5 (4)
O9—La1—H3B	110.0 (11)	C12—C11—C11^{i}	121.7 (4)
O4—La1—H3B	71.5 (16)	C11—C12—C13	120.3 (4)
O7—La1—H3B	62.3 (14)	C11—C12—H12	119.9
O12—La1—H3B	171.0 (7)	C13—C12—H12	119.9
H1A—O1—H1B	103 (2)	N6—C13—C12	124.5 (4)
H1A—O1—La1	128 (3)	N6—C13—H13	117.7
H1B—O1—La1	129 (2)	C12—C13—H13	117.7
H1B—O1—H1A	103 (2)	N6—C14—C15	123.4 (3)
La1—O1—H1A	128 (3)	N6—C14—H14	118.3
H1A—O1—H1B	103 (2)	C15—C14—H14	118.3
La1—O1—H1B	129 (2)	C11—C15—C14	120.2 (3)
H1A—O1—H1B	103 (2)	C11—C15—H15	119.9
La1—O2—H2A	128 (3)	C14—C15—H15	119.9
La1—O2—H2B	124 (3)	C17—C16—C20	116.6 (3)
H2A—O2—H2B	109 (2)	C17—C16—C16^{ii}	122.2 (4)
La1—O3—H3A	156 (5)	C20—C16—C16^{ii}	121.2 (4)
La1—O3—H3B	84 (5)	C18—C17—C16	119.4 (4)
H3A—O3—H3B	107 (6)	C18—C17—H17	120.3
N1—O4—La1	94.54 (16)	C16—C17—H17	120.3
N1—O6—La1	97.49 (15)	N7—C18—C17	125.0 (4)
N2—O7—La1	95.61 (16)	N7—C18—H18	117.5
N2—O9—La1	96.67 (19)	C17—C18—H18	117.5
N3—O10—La1	96.55 (18)	N7—C19—C20	124.5 (4)
N3—O12—La1	95.64 (18)	N7—C19—H19	117.7
O5—N1—O4	122.5 (3)	C20—C19—H19	117.7
O5—N1—O6	120.9 (3)	C19—C20—C16	119.7 (4)
O4—N1—O6	116.6 (2)	C19—C20—H20	120.2
O8—N2—O7	120.7 (3)	C16—C20—H20	120.2
O8—N2—O9	122.4 (3)		

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) −*x*, −*y*, −*z*.

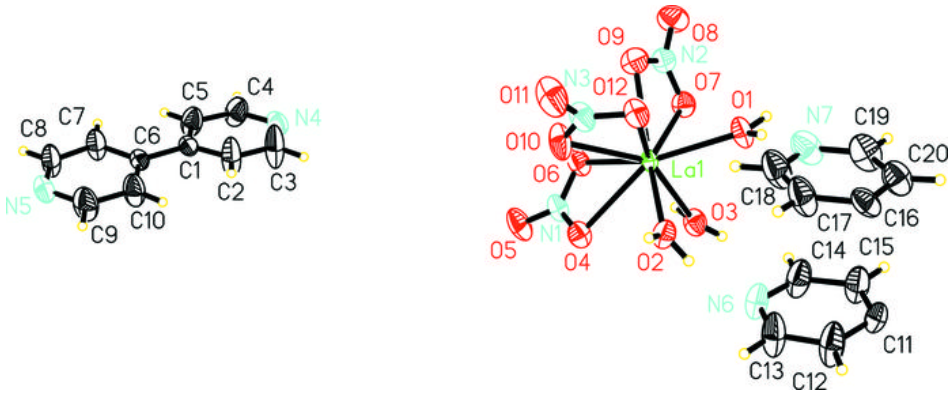
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2B···N6	0.86 (4)	1.84 (4)	2.668 (4)	161 (5)
O1—H1A···N7	0.87 (3)	1.87 (3)	2.736 (4)	173 (5)

O1—H1B···N5^{iii}	0.88 (3)	1.87 (3)	2.747 (3)	172 (4)
O3—H3A···N4^{iv}	0.86 (5)	2.08 (6)	2.684 (3)	128 (6)
O2—H2A···O8^{v}	0.86 (3)	2.21 (2)	3.002 (4)	154 (5)

Symmetry codes: (iii) *x*, *y*−1, *z*; (iv) −*x*+2, −*y*+1, −*z*+1; (v) *x*−1/2, −*y*+1/2, *z*−1/2.

Fig. 1


C5
C4
C8
C7
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N4
C1
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C3
N5
C10
C9
09
08
N2
N3
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07
011
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N7
C19
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La1
C20
06
C18
03
C17
C16
05
N1
04
02
C14
C15
N6
C11
C13
C12

Fig. 2